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L. HYVÄRINEN

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CONTENTS

	Page
Introduction	5
Theory	6
Template	13
Inversion	15
Bibliography	19

INTRODUCTION

The method described below provides an easy and inexpensive way to evaluate the Fourier series coefficients for an empirical function. The computation is carried out by taking the values of the function f(x) at certain values of x multiplied alternately by +1 or -1 and followed by summation. No weighting coefficients are needed, which facilitates the computation. The points x, at which the value of the function is needed, however, vary from one harmonic to another. Therefore it is preferable to plot the function at a certain scale and use a transparent template for finding these points for each harmonic.

In all numerical methods for Fourier analysis, the higher harmonics have a disturbing effect on the results. This is displayed here so that the coefficient of the n:th harmonic contains all the harmonics 6 nm $\pm$1. (m = 1, 2, 3...). If, however, the whole Fourier spectrum is calculated, the results are easily corrected for these higher harmonics, this in particular if the series converge rapidly.

THEORY

The real and imaginary parts of the exponential Fourier transform F (h) of function f (x)

$$(1)\quad \begin{cases} \mathfrak{F}[f(x)] = F(h) = \int_{-\infty}^{\infty} f(x)\, e^{-2\pi i h x}\, dx \\ \mathfrak{F}^{-1}[F(h)] = f(x) = \int_{-\infty}^{\infty} F(h)\, e^{+2\pi i h x}\, dh = [F(-h)] \end{cases}$$

can be expressed as

$$(2)\quad \begin{cases} \mathrm{Re}\, F(h) = F_e(h) = \int_{-\infty}^{\infty} f_e(x) \cos 2\pi h x\, dx \\ \mathrm{Im}\, F(h) = F_o(h) = -\int_{-\infty}^{\infty} f_o(x) \sin 2\pi h x\, dx \end{cases}$$

where f_e and f_o are the even and odd parts of f.

$$(3)\quad \begin{cases} f_e(x) = \tfrac{1}{2}\left[f(x) + f(-x)\right] \\ f_o(x) = \tfrac{1}{2}\left[f(x) - f(-x)\right] \end{cases} ; \quad \begin{cases} f_e(x) = f_e(-x) \\ f_o(x) = -f_o(-x) \end{cases} ; \quad \begin{cases} f_e(x) + f_o(x) = f(x) \\ f_e(x) - f_o(x) = f(-x) \end{cases}$$

The two following operators are also needed in the derivation 1)

$$(4)\quad \begin{cases} \operatorname{rep}_t f(x) = \sum_{\nu=-\infty}^{\infty} f(x - \nu t) \\ \operatorname{comb}_t f(x) = \sum_{\nu=-\infty}^{\infty} f(\nu t)\,\delta(x - \nu t) = f(x)\operatorname{rep}_t \delta(x) \end{cases}$$

$\delta(x)$ is the Dirac deltafunction and t is a constant parameter. Operators (4), when transformed, yield two important relationships 1)

$$(5)\quad \begin{cases} \mathfrak{F}\left[\operatorname{rep}_t f(x)\right] = \frac{1}{t}\operatorname{comb}_{\frac{1}{t}} F(h) \\ \mathfrak{F}\left[\operatorname{comb}_t f(x)\right] = \frac{1}{t}\operatorname{rep}_{\frac{1}{t}} F(h) \end{cases}$$

Same equations hold also for the inverse transformation. In (5) let $t = 1/n$ and $f(x) = f_e(x)$ or $f(x) = f_o(x)$. We obtain when both sides are divided through by n

$$\frac{1}{n}\,\mathfrak{F}\left[\operatorname{rep}_{\frac{1}{n}} f_e(x)\right] = \operatorname{comb}_n F_e(h) = \sum_{\nu=-\infty}^{\infty} F_e(n\nu)\,\delta(h-n\nu)$$

(6)

$$\frac{1}{n}\,\mathfrak{F}\left[\operatorname{rep}_{\frac{1}{n}} f_o(x)\right] = i\operatorname{comb}_n F_o(h) = \sum_{\nu=-\infty}^{\infty} iF_o(n\nu)\,\delta(h-n\nu)$$

Obviously spectra (6) are discrete with δ-peaks at each multiple of n. If expressions similar to (6), but $t = 1/2\ n$, are written down, they have δ-peaks only at even multiples of n. The difference of these two expressions thus leaves the odd multiples of n.

(7)
$$\begin{cases} \frac{1}{2n}\,\mathfrak{F}\left[2\operatorname{rep}_{\frac{1}{n}} f_e(x) - \operatorname{rep}_{\frac{1}{2n}} f_e(x)\right] = \sum_{\nu\ \text{odd}} F_e(n\nu)\,\delta(h-n\nu) \\ \frac{1}{2n}\,\mathfrak{F}\left[2\operatorname{rep}_{\frac{1}{n}} f_o(x) - \operatorname{rep}_{\frac{1}{2n}} f_o(x)\right] = \sum_{\nu\ \text{odd}} iF_o(n\nu)\,\delta(h-n\nu) \end{cases}$$

Using the transformation

(8) $$\mathfrak{F}\left[e^{+2\pi i n\nu x}\right] = \delta(h-n\nu)$$

and properties

(9) $$F_e(h) = F_e(-h)\,;\quad F_o(h) = -F_o(-h)$$

for a real function $f(x)$ equations (7) give

$$(10)\quad \begin{cases} g_e(x) \equiv \frac{1}{2n}\left[2\,\mathrm{rep}_{\frac{1}{n}} f_e(x) - \mathrm{rep}_{\frac{1}{2n}} f_e(x)\right] = 2\sum\limits_{\substack{\nu>0\\ \text{odd}}} F_e(n\nu)\cos 2\pi n\nu x \\ g_o(x) \equiv \frac{1}{2n}\left[2\,\mathrm{rep}_{\frac{1}{n}} f_o(x) - \mathrm{rep}_{\frac{1}{2n}} f_o(x)\right] = -2\sum\limits_{\substack{\nu>0\\ \text{odd}}} F_o(n\nu)\sin 2\pi n\nu x \end{cases}$$

Let further $p(x)$ be a periodic function with period equal to unity and let us denote by $f(x)$ the function that is equal to $p(x)$ over one period and zero elsewhere.

$$(11)\qquad f(x) = \begin{cases} p(x) & \text{when } -\tfrac{1}{2} < x \le \tfrac{1}{2} \\ 0 & \text{when } x \le -\tfrac{1}{2} \text{ or } x > \tfrac{1}{2} \end{cases}$$

Now the Fourier series coefficients a_n and b_n of $p(x)$ are

$$(12)\quad \begin{cases} a_n = 2\int\limits_{-\frac{1}{2}}^{\frac{1}{2}} p(x)\cos 2\pi n x\,dx = 2\int\limits_{-\infty}^{\infty} f_e(x)\cos 2\pi n x\,dx \\ b_n = 2\int\limits_{-\frac{1}{2}}^{\frac{1}{2}} p(x)\sin 2\pi n x\,dx = 2\int\limits_{-\infty}^{\infty} f_o(x)\sin 2\pi n x\,dx \end{cases}$$

where f_e and f_o are now the even and odd parts of (11). By equations (2) we have

$$(13)\quad \begin{cases} a_n = 2F_e(n) \\ b_n = -2F_o(n) \end{cases} \qquad n \ge 0$$

and finally from (10) and (13)

$$(14)\quad \begin{cases} g_e(x) = a_n \cos 2\pi nx + a_{3n} \cos 2\pi 3nx + a_{5n} \cos 2\pi 5nx + \dots \\ g_o(x) = b_n \sin 2\pi nx + b_{3n} \sin 2\pi 3nx + b_{5n} \sin 2\pi 5nx + \dots \end{cases}$$

Finding suitable values for x in g_e and g_o we can still eliminate all coefficients whose subscripts are divisible by 3n. These turn out to be $x = 1/12n$ for g_e and $x = 1/6n$ for g_o. Thus

$$(15)\quad \begin{cases} g_e\left(\frac{1}{12n}\right) = \frac{\sqrt{3}}{2}\left[a_n - a_{5n} - a_{7n} + a_{11n} + a_{13n} - \dots\right] \\ g_o\left(\frac{1}{6n}\right) = \frac{\sqrt{3}}{2}\left[b_n - b_{5n} + b_{7n} - b_{11n} + b_{13n} - \dots\right] \end{cases}$$

By equations (10) and (4) equations (15) can be worked out to yield

$$(16)\quad \begin{cases} \frac{1}{n\sqrt{3}} \sum_{\nu=-\infty}^{\infty} (-1)^\nu f_e\left(\frac{1-6\nu}{12n}\right) = a_n - a_{5n} - a_{7n} + a_{11n} + a_{13n} - \dots \\ \frac{1}{n\sqrt{3}} \sum_{\nu=-\infty}^{\infty} (-1)^\nu f_o\left(\frac{1-3\nu}{6n}\right) = b_n - b_{5n} + b_{7n} - b_{11n} + b_{13n} - \dots \end{cases}$$

The range of summation from $-\infty$ to ∞ is only formal, for by definition (11) f(x) is zero outside the interval $(-1/2,\ 1/2)$ and the sums contain actyally only 2n terms.

According to equations (16) the coefficients a_n and b_n of successive harmonics of periodic function p(x) are calculated in the following way: We take one period of the

function according to (11) and find the even and odd parts of it (3). Next we find the points $(1-6\nu)/12n$ or $(1-3\nu)6n$ respectively and evaluate the sums (16) for $n = 1, 2, 3 \cdots N$ until the series converge to a value small enough in comparison with the accuracy required. And finally the coefficients obtained in this way can be corrected for the higher harmonics $5n$, $7n$, $11n$, etc.

Even the zero order harmonic a_0 can be evaluated by this method. This can be accomplished in two different ways: Obviously the value of $p(x)$ or $f(x)$ at the origin is

$$(17) \qquad p(o) = f(o) = \tfrac{1}{2} a_0 + \sum_{\nu=1}^{\infty} a_\nu$$

If the cosine series foefficients a_n $(n > 0)$ have been evaluated in the manner suggested above, we can easily compute the sum

$$\sum_{\nu=1}^{\infty} a_\nu .$$

Hence

$$(18) \qquad a_0 = 2\left[f(o) - \sum_{\nu=1}^{\infty} a_\nu\right]$$

Another way of finding a_0 is suggested by the first of equations (6).

By an inversion

$$\frac{1}{n} \operatorname{rep}_{\frac{1}{n}} f_e(x) = F_e(o) + 2 \sum_{\nu=1}^{\infty} F_e(n\nu) \cos 2\pi n \nu x$$

(19)

$$= \tfrac{1}{2} a_o + \sum_{\nu=1}^{\infty} a_{n\nu} \cos 2\pi n \nu x$$

If, within the limits of required accuracy, $a_n = 0$ for $n \geq n_o$,

$$\frac{1}{n_o} \operatorname{rep}_{\frac{1}{n_o}} f_e(o) = \tfrac{1}{2} a_o + \sum_{\nu=1}^{\infty} a_{\nu n_o} = \tfrac{1}{2} a_o$$

or

(20)

$$a_o = \frac{2}{n_o} \operatorname{rep}_{\frac{1}{n_o}} f_e(o) = \frac{2}{n_o} \sum_{\nu=-\infty}^{\infty} f_e\left(\frac{\nu}{n_o}\right)$$

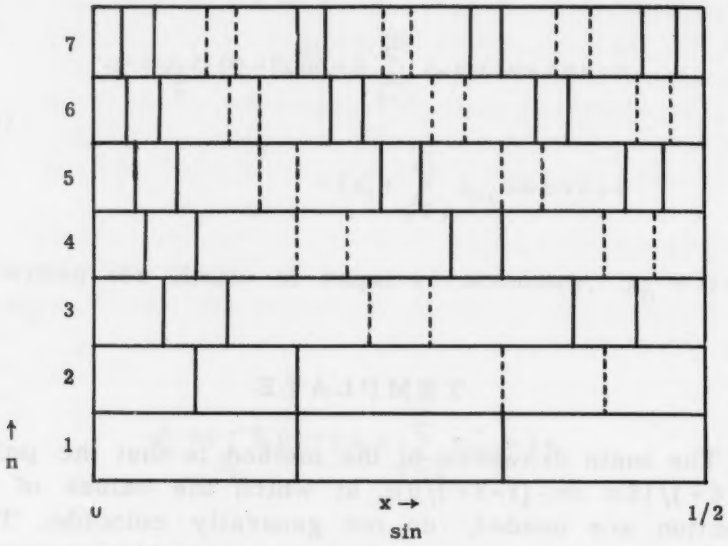
Keeping in mind equations (3) and (11), according to which $f_e(-1/2) = f_e(1/2) = \frac{1}{2} p(1/2)$, expression (20) turns out to be the trapezoidal rule for the integral of f_e the spacings of ordinates being equal to $1/n_o$.

TEMPLATE

The main drawback of the method is that the points $(1-6\nu)/12n$ or $(1-3\nu)/6n$, at which the values of the function are needed, do not generally coincide. This difficulty can be overcome by using a template engraved on a transparent sheet (lucite, celluloid, etc).

Two sheets, each having the breadth of one period, which has been standardized to, say, 40 cm, are divided by straight lines into horizontal strips. One of the sheets is used to the calculation of a_n, the other for b_n. On the first strip (corresponding to $n = 1$) of the a_n sheet are marked the points $(1-6\nu)/12$ with vertical lines extending across the strip, and the same procedure is repeated for each n on both sheets. The sign of each term is indicated by colouring the lines corresponding to positive (ν even) red and the negative (ν odd) black. Now, when $f_e(x)$ and $f_o(x)$ have been plotted on a plotting paper, the ordinates can be read easily by moving the templates up and down on the paper.

By using properties $f_e(x) = f_e(-x)$ and $f_o(x) = -f_o(-x)$ it suffices to make templates covering only half of the period. The points from the negative half of the period are shifted on the positive half with proper sign. On cosine template the signs are not altered, on sine template they are opposite. Fig. 1 depicts cosine and sine templates for $n = 1 - 7$.



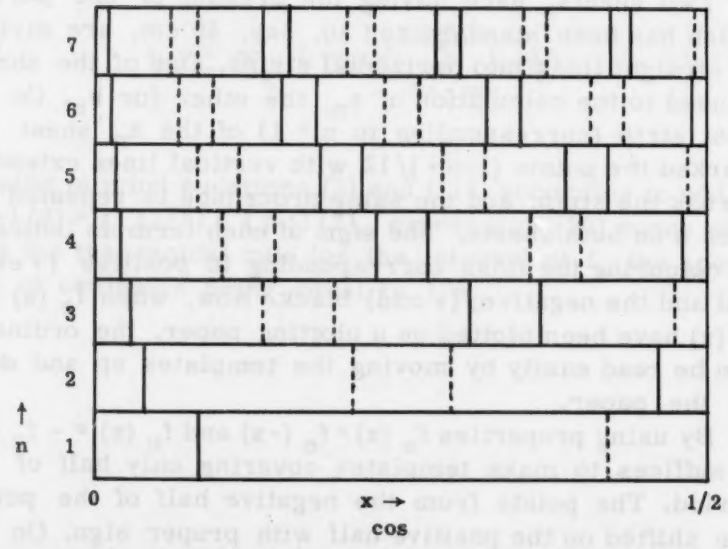


Fig. 1. Sine and cosine template for coefficients a_n and b_n, n = 1 - 7. Terms of positive sign have been drawn with continuous lines and those of negative sign with dashed lines.

INVERSION

In many instances, e.g. crystal analysis, we know the Fourier coefficients (a_n, b_n) and want to obtain the function p (x) or one period of it f (x). This problem can also be handled by the template method.

By equations (13) we have the real and imaginary part of the Fourier transform of f (x) at integral values n of h

$$(21) \quad \begin{cases} F_e(h) = R_e F(h) = \frac{1}{2} a_h & n = h = \text{integer} \geq o \\ F_o(h) = I_m F(h) = -\frac{1}{2} b_h & (b_o = o) \end{cases}$$

And, because ReF (h) is an even and ImF (h) an odd function, functions F_e and F_o can be extended to the negative values of h, too.

$$(22) \quad \begin{cases} F_e(-h) = \frac{1}{2} a_h & n = h = \text{integer} > o \\ F_o(-h) = \frac{1}{2} b_h \end{cases}$$

It is easily verified that the periodic function p (x) is an infinite repetition of one of its periods

(23) $$p(x) = \mathrm{rep}_1\, f(x)$$

but there is an infinite number of functions $f_k(x)$ which, when repeated at intervals 1, give the same function.

(24) $$p(x) = \mathrm{rep}_1\, f_k(x)$$

Among these f(x) is the "simplest" in the sense that the repetitions never operlap one another. Obviously both functions (23) and (24) must have the same series, or by (21) and (22) the transforms of f and f_k coincide at h = integer. At nonintegral values they may differ from one another. It follows from this property that by joining the points F (n) by an arbitrary (continuous) curve we get the transform F_k (h) of one of functions f_k (x).

One of the basic properties of Fourier transforms is

(25) $$\frac{1}{2m}\,\mathfrak{F}\left[f_k\left(\frac{x}{2m}\right)\right] = F_k(2mh) \qquad m = \text{constant}$$

or by the second of equations (1)

(26) $$\mathfrak{F}\left[F_k(-2mh)\right] = \frac{1}{2m}\, f_k\left(\frac{x}{2m}\right)$$

Function F_k (-2 mh) is aperiodic but becomes periodic by operation

(27) $$P(h) = \mathrm{rep}_1\, F_k(-2mh) = P_e(h) + iP_o(h)$$

In analogy with (24) the transform of P (h) coincides with that of F (-2 mh) at points x = integer. Or by (13)

$$\begin{cases} f_{k_e}\left(\frac{\nu}{2m}\right) = 2\,a_\nu \\ f_{k_o}\left(\frac{\nu}{2m}\right) = -2\,b_\nu \qquad \nu = \text{integer} \geq 0 \end{cases}$$

(28)

$$\begin{cases} f_{k_e}\left(\frac{-\nu}{2m}\right) = 2\,a_\nu \\ f_{k_o}\left(\frac{-\nu}{2m}\right) = 2\,b_\nu \end{cases}$$

where a_ν and b_ν are the cos and sin series coefficients of P_e (h) and P_o (h) and f_{ke} and f_{ko} are the even and odd parts of f_k. Finally

$$f_k\left(\frac{\nu}{2m}\right) = 2 \begin{cases} a_\nu - b_\nu & \nu \geq o \\ a_\nu + b_\nu & \nu < o \end{cases} \tag{29}$$

and by (24)

$$p\left(\frac{\nu}{2m}\right) = \sum_\mu f_k\left(\frac{\nu}{2m} - \mu\right) = \text{rep}_1\, f_k\left(\frac{\nu}{2m}\right) \tag{30}$$

In this way 2 m points of p (x) are obtained to the period. It can be shown by a detailed discussion that if the coefficients a_n, b_n are known up to the N:th harmonic, the best accuracy in p (x) is obtained by taking m = N. A higher value of m gives more points to the period but they do not improve the detail in p (x). If on the other

hand $m < N$, the points $\nu/2m$ are too far apart giving a poorer detail and some of the information is lost.

The degree of overlapping of functions f_k in (30) depends essentially on the smoothness of the curve by which the points $F(2nm)$ are joined. The smoother curve gives less overlap. Theoretically, if the interpolation is done with Hadamard's [2] interpolation formula

$$(31) \qquad F_k(2mh) = \sum_{n=-\infty}^{\infty} F(2nm) \frac{\sin 2\pi m(h-n)}{2\pi m(h-n)}$$

no overlap occurs [3]. In practice a smooth hand-drawn curve approximates very well this function.

In practice, then, the inversion is done by dividing the half period into N equal parts ($m = N$) and plotting the coefficients a_n and b_n at the points of division. Then the points are respectively joined with a smooth curve and analysed with the template. The possible overlapping is corrected by equation (30).

Theoretically there are no limits as to how high harmonics can be analyzed in this way, but the work needed for each harmonic grows in proportion to n, since there are $2n$ terms to add.

A detailed analysis indicates that if all the ordinates in (16) are read with a certain accuracy $\pm \Delta$, the error in a_n and b_n is approximately $\pm \Delta / \sqrt{n}$. This means that the higher harmonics are more accurate than the lower ones in the absolute sense.

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